HW6

```
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
```

```
Note: Accessing on-line PDB file
```

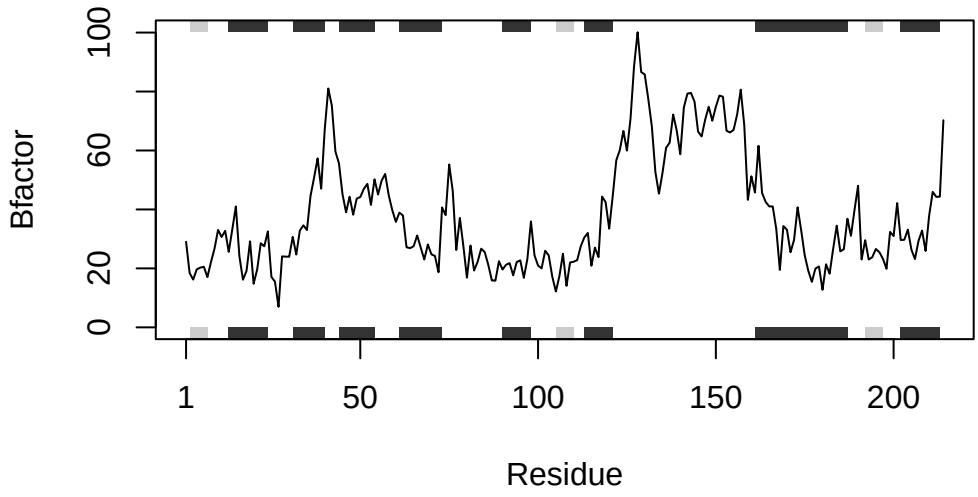
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

```
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
```

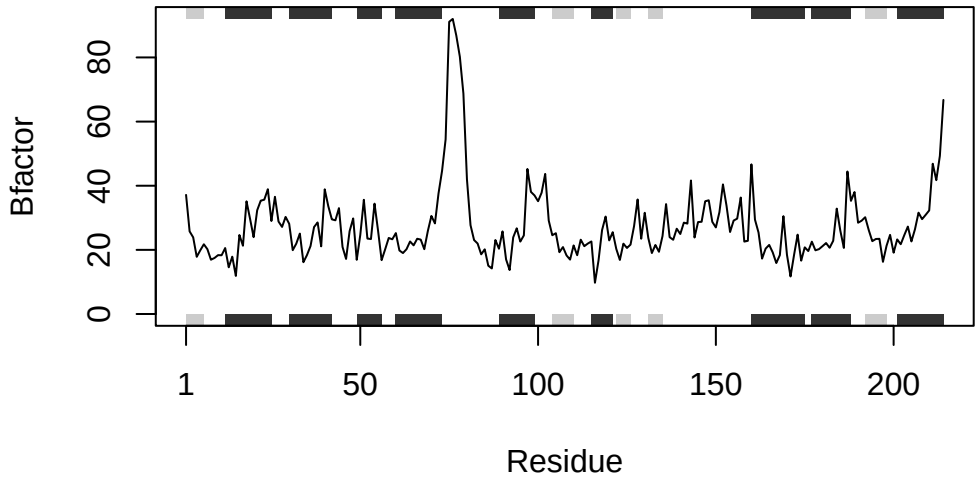
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

```
Note: Accessing on-line PDB file
```

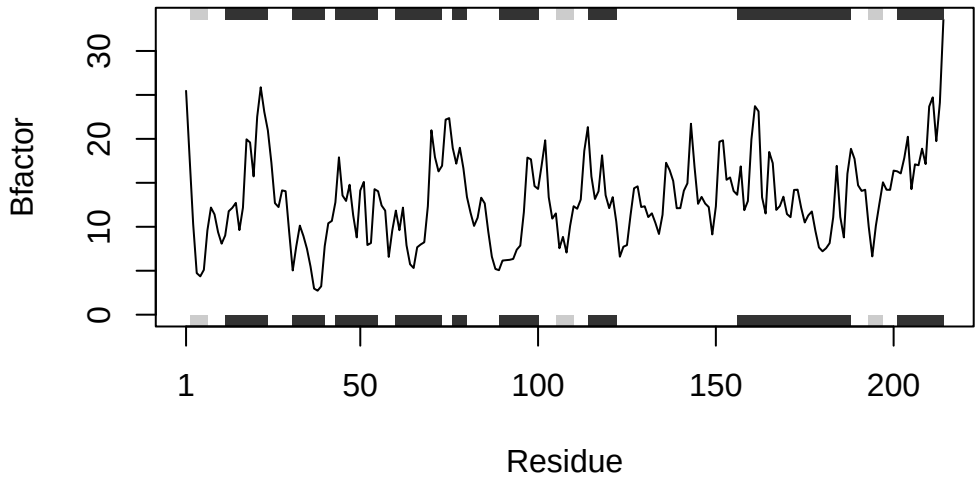
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```




```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



Q1. What type of object is returned from the read.pdb() function?

```
class(s1)
```

```
[1] "pdb" "sse"
```

PDB structure object

Q2. What does the trim.pdb() function do?

It reduces pdb to a smaller pdb object that only contains a subset of chain and type

Q3. What input parameter would turn off the marginal black and grey rectangles in the plots and what do they represent in this case?

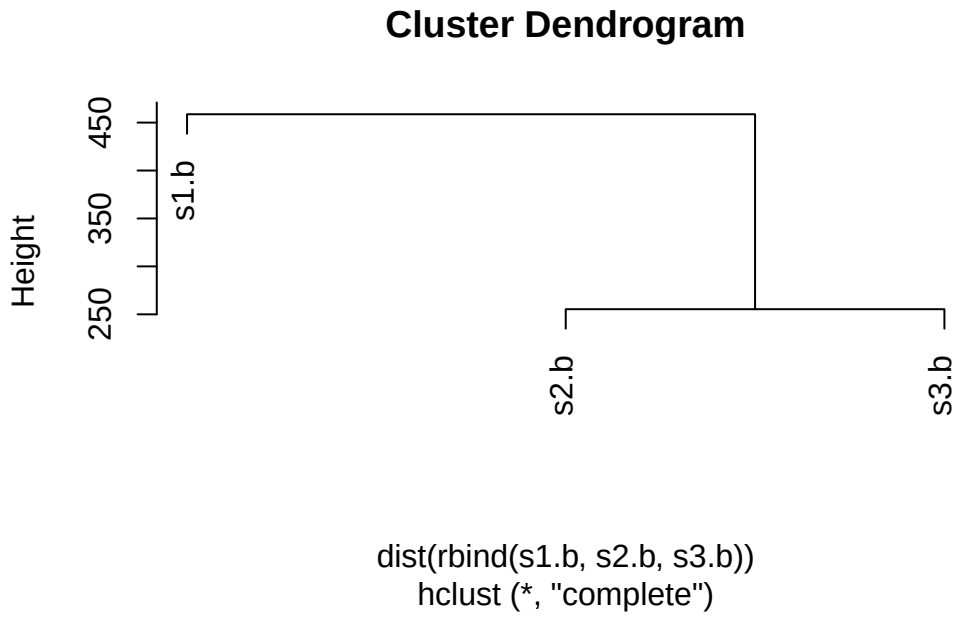
sse parameter would turn off the rectangles and they represent secondary structure elements(black: alpha helices; light grey: beta sheets)

Q4. What would be a better plot to compare across the different proteins?

Plots that can show sequence and structural conservation, for example structural superposition diagram or alignment graphs

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this?

```
hc <- hclust( dist( rbind(s1.b, s2.b, s3.b) ) )
plot(hc)
```



s2 and s3 are more similar, height is used to quantify them also the joint between s2 and s3 show that they are more closely related

Write a function

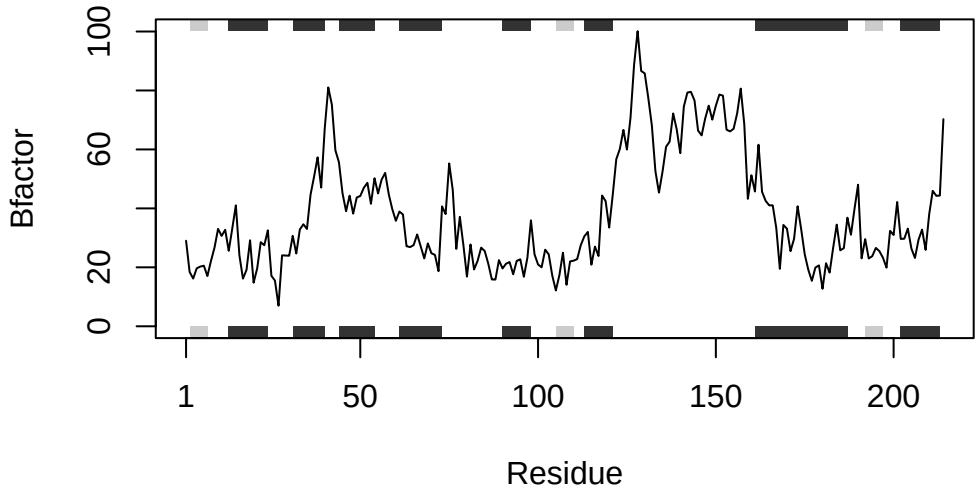
Q6. How would you generalize the original code above to work with any set of input protein structures?

```
pdbanalysis <- function(x){
    s <- read.pdb(x)
    s.chainA <- trim.pdb(s, chain="A", elety="CA")
    s.b <- s.chainA$atom$b
    plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
    return(s.b)

  }
```

1. Input of the function is the pdb structure object(pdb file)
2. The function is to asccess the pdb file, reduce it to specific and desired chain to analyze a given kinase
3. The output is to plot residue number vs B-factor with noted secondary structure elements

```
pdbanalysis ("4AKE")
```

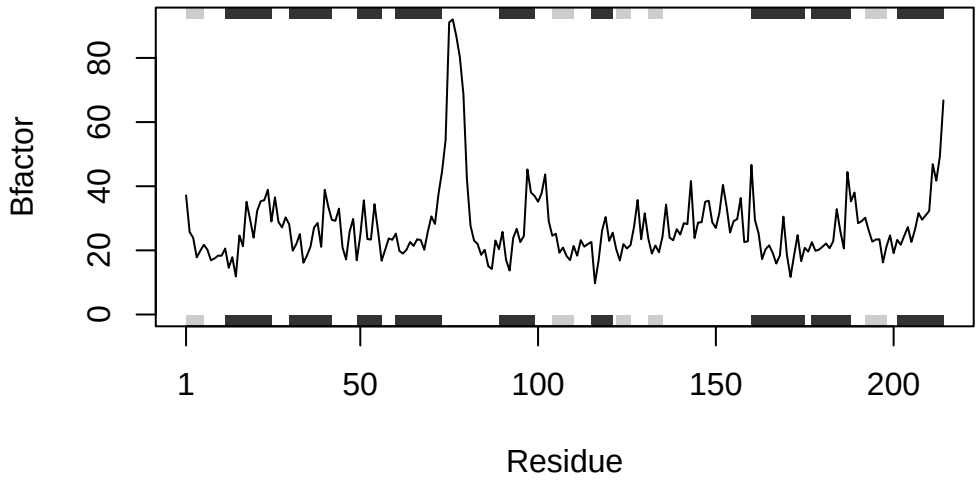
```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/b2/
gd_q_gjx2596x8rky5bhvvfh0000gn/T//RtmpTFSb5c/4AKE.pdb exists. Skipping download
```




```
  [1]  29.02  18.44  16.20  19.67  20.26  20.55  17.05  22.13  26.71  33.05
 [11]  30.66  32.73  25.61  33.19  41.03  24.09  16.18  19.14  29.19  14.79
 [21]  19.63  28.54  27.49  32.56  17.13  15.50   6.98  24.07  24.00  23.94
 [31]  30.70  24.70  32.84  34.60  33.01  44.60  50.74  57.32  47.04  67.13
 [41]  81.04  75.20  59.68  55.63  45.12  39.04  44.31  38.21  43.70  44.19
 [51]  47.00  48.67  41.54  50.22  45.07  49.77  52.04  44.82  39.75  35.79
 [61]  38.92  37.93  27.18  26.86  27.53  31.16  27.08  23.03  28.12  24.78
 [71]  24.22  18.69  40.67  38.08  55.26  46.29  26.25  37.14  27.50  16.86
 [81]  27.76  19.27  22.22  26.70  25.52  21.22  15.90  15.84  22.44  19.61
 [91]  21.23  21.79  17.64  22.19  22.73  16.80  23.25  35.95  24.42  20.96
[101]  20.00  25.99  24.39  17.19  12.16  17.35  24.97  14.08  22.01  22.26
[111]  22.78  27.47  30.49  32.02  20.90  27.03  23.84  44.37  42.47  33.48
[121]  44.56  56.67  60.18  66.62  59.95  70.81  88.63 100.11  86.60  85.80
[131]  77.48  68.13  52.66  45.34  52.43  60.90  62.64  72.19  66.75  58.73
[141]  74.57  79.29  79.53  76.58  66.40  64.76  70.48  74.84  70.11  74.82
[151]  78.61  78.24  66.70  66.10  67.01  72.28  80.64  68.54  43.23  51.24
[161]  45.72  61.60  45.61  42.57  41.03  41.02  33.34  19.48  34.38  33.11
[171]  25.48  29.68  40.71  32.91  24.41  19.20  15.43  19.93  20.66  12.72
[181]  21.40  18.21  26.68  34.50  25.77  26.52  36.85  31.05  39.84  48.03
[191]  23.04  29.57  23.00  23.80  26.59  25.49  23.25  19.89  32.37  30.97
[201]  42.16  29.64  29.69  33.15  26.38  23.17  29.35  32.80  25.92  38.01
[211]  45.95  44.26  44.35  70.26
```

```
pdbanalysis ("1AKE")
```

```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/b2/
gd_q_gjx2596x8rky5bhvvfh0000gn/T//RtmpTFSb5c/1AKE.pdb exists. Skipping download

   PDB has ALT records, taking A only, rm.alt=TRUE
```

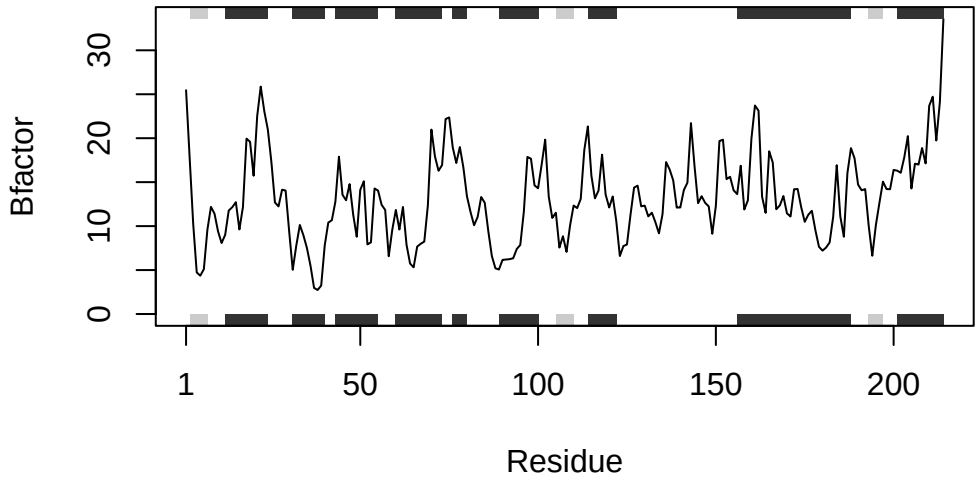



```
  [1] 37.14 25.76 23.90 17.83 19.86 21.75 20.21 16.92 17.47 18.35 18.31 20.57
 [13] 14.56 17.87 11.87 24.63 21.29 35.13 29.68 23.96 32.34 35.34 35.64 38.91
 [25] 29.00 36.55 28.83 27.15 30.28 28.13 19.90 21.95 25.07 16.15 18.35 21.19
 [37] 27.13 28.55 21.10 38.88 33.63 29.51 29.21 33.01 20.92 17.17 25.84 29.80
 [49] 16.89 24.66 35.62 23.52 23.37 34.41 25.96 16.79 20.20 23.72 23.29 25.23
 [61] 19.81 19.00 20.21 22.62 21.40 23.47 23.20 20.21 25.90 30.58 28.25 37.60
 [73] 44.66 54.46 91.10 92.02 86.85 80.21 68.72 42.01 27.69 23.06 21.98 18.60
 [85] 20.17 15.06 14.20 23.07 20.36 25.76 17.02 13.71 23.88 26.72 22.58 24.51
 [97] 45.23 38.07 36.97 35.17 37.83 43.69 29.14 24.56 25.20 19.27 20.88 18.27
[109] 16.96 21.38 18.33 23.18 21.15 21.97 22.63  9.74 16.71 26.18 30.39 22.95
[121] 25.51 20.28 16.86 21.94 20.59 21.64 27.42 35.72 23.47 31.57 23.71 19.01
[133] 21.52 19.40 24.32 34.28 23.96 23.14 26.60 24.94 28.49 28.18 41.64 23.85
[145] 28.67 28.76 35.16 35.46 28.74 26.99 31.74 40.41 33.73 25.57 29.13 29.74
[157] 36.32 22.58 22.82 46.67 29.44 25.40 17.27 20.38 21.55 19.19 15.89 18.37
[169] 30.51 18.47 11.70 18.45 24.75 16.63 20.80 19.62 22.56 19.87 20.22 21.16
[181] 22.13 20.66 22.82 32.86 26.04 20.60 44.44 35.28 38.03 28.46 29.10 30.19
[193] 26.17 22.71 23.39 23.44 16.27 21.26 24.67 19.12 23.26 21.75 24.59 27.26
[205] 22.63 26.40 31.60 29.57 30.90 32.29 46.86 41.73 49.31 66.76
```

```
pdbanalysis ("1E4Y")
```

```
  Note: Accessing on-line PDB file
```

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/b2/
gd_q_gjx2596x8rky5bhvvfh0000gn/T//RtmpTFSb5c/1E4Y.pdb exists. Skipping download
```




```
  [1] 25.46 17.86 10.28  4.73  4.36  5.10  9.59 12.19 11.41  9.39  8.08  9.01
 [13] 11.77 12.15 12.72  9.62 12.18 19.95 19.59 15.73 22.51 25.87 23.08 20.97
 [25] 17.28 12.69 12.24 14.14 14.05  9.38  5.03  7.78 10.13  8.96  7.50  5.48
 [37]  2.97  2.73  3.23  7.81 10.40 10.67 12.79 17.90 13.56 12.94 14.78 11.31
 [49]  8.79 14.13 15.10  7.92  8.15 14.28 14.04 12.42 11.84  6.57  9.59 11.84
 [61]  9.61 12.18  7.89  5.74  5.31  7.67  7.99  8.24 12.34 20.98 17.93 16.30
 [73] 16.94 22.19 22.36 18.96 17.18 18.99 16.65 13.39 11.61 10.10 11.03 13.31
 [85] 12.66  9.44  6.60  5.20  5.06  6.16  6.20  6.24  6.34  7.39  7.86 11.66
 [97] 17.87 17.67 14.63 14.30 16.98 19.84 13.36 10.93 11.52  7.56  8.85  7.07
[109] 10.08 12.34 12.05 13.10 18.63 21.34 15.73 13.16 14.04 18.13 13.59 12.12
[121] 13.37 10.57  6.60  7.73  7.91 11.31 14.38 14.60 12.25 12.33 11.10 11.53
[133] 10.44  9.18 11.36 17.28 16.45 15.21 12.11 12.12 14.10 14.94 21.72 16.82
[145] 12.61 13.40 12.64 12.24  9.13 12.31 19.68 19.83 15.34 15.61 14.07 13.64
[157] 16.87 11.89 12.92 19.93 23.72 23.13 13.35 11.51 18.51 17.24 11.92 12.36
[169] 13.42 11.45 11.09 14.19 14.22 12.15 10.49 11.29 11.74  9.53  7.65  7.21
[181]  7.56  8.14 11.07 16.93 11.12  8.79 16.03 18.87 17.72 14.72 14.08 14.21
[193]  9.99  6.63 10.11 12.64 15.06 14.21 14.20 16.39 16.31 16.07 17.83 20.24
[205] 14.28 17.10 17.00 18.88 17.13 23.68 24.72 19.74 24.12 33.57
```